3-(Benzoylamino) thiophane

Inchi: InChI=1S/C11H13NOS/c13-11(9-4-2-1-3-5-9)12-10-6-7-14-8-10/h1-5,10H,6-8H2,(H,12,1
InchiKey: DONJDQMILBHKEB-UHFFFAOYSA-N
Formula: C11H13NOS
SMILES: OC(=NC1CCSC1)c1ccccc1
Mol. weight [g/mol]: 207.29
CAS: 92367-69-6

Physical Properties

Property code	Value	Unit	Source
hf	-7.90	kJ/mol	Joback Method
hvap	68.50	kJ/mol	Joback Method
log10ws	-2.51		Crippen Method
logp	2.497		Crippen Method
mcvol	159.130	ml/mol	McGowan Method
pc	3166.83	kPa	Joback Method
tb	709.61	K	Joback Method
tc	955.15	K	Joback Method

Sources

Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws
Joback Method: https://en.wikipedia.org/wiki/Joback_method
McGowan Method: http://link.springer.com/article/10.1007/BF02311772
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C92367696&Units=SI

Legend

hf: Enthalpy of formation at standard conditions
hvap: Enthalpy of vaporization at standard conditions
log10ws: Log10 of Water solubility in mol/l

logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature